PATENT COOPERATION TREATY REC'D 2 6 JUL 2006 From the INTERNATIONAL SEARCHING AUTHORITY To: WRITTEN OPINION OF THE see form PCT/ISA/220 INTERNATIONAL SEARCHING AUTHORITY (PCT Rule 43*bis*.1) Date of mailing (day/month/year) see form PCT/ISA/210 (second sheet) Applicant's or agent's file reference FOR FURTHER ACTION see form PCT/ISA/220 See paragraph 2 below International application No. International filing date (day/month/year) Priority date (day/month/year) PCT/EP2005/002114 25.02.2005 19.03.2004 International Patent Classification (IPC) or both national classification and IPC INV. G06F17/14 G01J3/45 Applicant THERMO ELECTRON CORPORATION This opinion contains indications relating to the following items: Box No. I Basis of the opinion ☐ Box No. II **Priority** ☐ Box No. III Non-establishment of opinion with regard to novelty, inventive step and industrial applicability ☐ Box No. IV Lack of unity of invention ☑ Box No. V Reasoned statement under Rule 43bis.1(a)(i) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement ☐ Box No. VI Certain documents cited ☐ Box No. VII Certain defects in the international application Box No. VIII Certain observations on the international application **FURTHER ACTION** If a demand for international preliminary examination is made, this opinion will usually be considered to be a written opinion of the International Preliminary Examining Authority ("IPEA") except that this does not apply where the applicant chooses an Authority other than this one to be the IPEA and the chosen IPEA has notifed the International Bureau under Rule 66.1bis(b) that written opinions of this International Searching Authority will not be so considered. If this opinion is, as provided above, considered to be a written opinion of the IPEA, the applicant is invited to submit to the IPEA a written reply together, where appropriate, with amendments, before the expiration of 3 months from the date of mailing of Form PCT/ISA/220 or before the expiration of 22 months from the priority date, whichever expires later. For further options, see Form PCT/ISA/220. For further details, see notes to Form PCT/ISA/220. Name and mailing address of the ISA:

European Patent Office - Gitschiner Str. 103 D-10958 Berlin

Tel. +49 30 25901 - 0 Fax: +49 30 25901 - 840 Date of completion of this opinion

see form PCT/ISA/210 **Authorized Officer**

Domingo Vecchioni, M

Telephone No. +49 30 25901-666



International application No. PCT/EP2005/002114

_					
_	Во	x N	p. I Basis of the opinion		
1	. With regard to the language, this opinion has been established on the basis of:				
	X	the	e international application in the language in which it was filed		
		a t pu	ranslation of the international application into , which is the language of a translation furnished for the rposes of international search (Rules 12.3(a) and 23.1 (b)).		
2. With regard to any nucleotide and/or amino acid sequence disclosed in the international application are necessary to the claimed invention, this opinion has been established on the basis of:					
	a. t	ype	of material:		
	ļ		a sequence listing		
			table(s) related to the sequence listing		
	b. f	orm	at of material:		
	ĺ		on paper		
	l		in electronic form		
	c. ti	ime	of filing/furnishing:		
	[contained in the international application as filed.		
	í		filed together with the international application in electronic form.		
	[furnished subsequently to this Authority for the purposes of search.		
3.		cop	addition, in the case that more than one version or copy of a sequence listing and/or table relating thereto been filed or furnished, the required statements that the information in the subsequent or additional lies is identical to that in the application as filed or does not go beyond the application as filed, as propriate, were furnished.		
4	Additional comments				

International application No. PCT/EP2005/002114

Box No. V Reasoned statement under Rule 43bis.1(a)(i) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement

1. Statement

Novelty (N)

Yes: Claims

5,6

No: Claims

1-4,7-13

Inventive step (IS)

Yes: Claims

No: Claims

1-13

Industrial applicability (IA)

Yes: Claims

1-13

No: Claims

2. Citations and explanations

see separate sheet

Re Item V

Reasoned statement with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement

- The following documents are cited in the International Search Report:
 - D1: R.T. Pajer and I.M. Armitage: "A method for complex interpolation of spectral segments", *Journal of Magnetic Resonance*, vol. 21, no. 3, March 1976, pages 485-489. [XP002390699]
 - D2: T. Kupka, J. Pacha, and J.O. Dziegielewski: "Application of data processing for sensitivity and resolution enhancement of 31P and 13C NMR spectra of humic substances", *Magnetic Resonance in Chemistry*, vol. 27, no. 1, 1989, pages 21-26. [XP002390700]
 - D3: K. Roth and B. Kirste: "Application of Fourier transformation techniques for sensitivity and resolution enhancement of continuous wave EPR spectra" *Journal of Magnetic Resonance*, vol. 63, no. 2, 15 June 1985, pages 360-364. [XP002390701]
 - D4: J.C. Lindon and A.G. Ferrige: "Digitisation and data processing in Fourier transform NMR", Progress in Nuclear Magnetic Resonance Spectroscopy, vol. 14, 1980, pages 27-66. [XP002390702]
 - D5: Z. Zolnai, J. Juranic, J.L. Markley, and S. Macura: "Zooming, a practical strategy for improving the quality of multidimensional NMR spectra" *Journal of Magnetic Resonance, Series A*, vol. 119, no. 1, March 1996, pages 53-64. [XP002390703]
 - D6: T.J. Francl, R.L. Hunter, and R.T. McIver, Jr. "Zoom transform for mass measurement accuracy in Fourier transform mass spectrometry", *Analytical Chemistry*, vol. 55, no. 13, November 1983, pages 2094-2096. [XP002390704]
 - D7: I. Pelczer and S. Szalma: "Multidimensional NMR and data processing" *Chemical Reviews*, vol. 91, no. 7, November 1991, pages 1507-1524. [XP002390705]

In this communication, reference is made to documents D1 and D6.

The subject matter of claims 1 to 4 and 7 to 13 is not new in the sense of Article 33(2) PCT.
 The subject matter of claims 5 and 6 appears to be new (Article 33(2) PCT) but does not involve an inventive step in the sense of Article 33(3) PCT.

2.1 Document D1

In the wording of the present application, D1 discloses a method (see in particular last paragraph of page 487: the "second method") of enhancing spectral data (see abstract: FT

WRITTEN OPINION OF THE INTERNATIONAL SEARCHING AUTHORITY (SEPARATE SHEET)

International application No.

PCT/EP2005/002114

NMR spectra), said data comprising M discrete intensity values within a range of frequency values ("N point complex spectral segment"), said method comprising:

- applying a first function ("inverse complex transform") being a Fourier transform to the spectral data to obtain an inverse transform of the spectrum ("complex pseudo FID"),
- apodizing said inverse transform ("applying sensitivity or resolution enhancement as desired"; see also page 488, lines 21 to 23: "the pseudo FID is sensitivity enhanced by the function e^{-t/r}"),
- zero-filling the apodized inverse transform by a factor Z ("zero extend this pseudo FID by N or more complex points"), and
- applying a second function ("complex transform") to the zero-filled apodized inverse transform to obtain a spectrum comprsing N>M discrete intensities values within said range of frequencies ("interpolated complex spectral segment").

The method is implemented in NMR computer systems (see abstract).

Hence, having regard to the disclosure of D1, the subject matter of claims 1 to 4 and 8 to 13 is not new (Article 33(2) PCT).

The method of D1 is applied to FT NMR spectra. However, it would obvious to a skilled person to use the same method for other kind of spectra, as the ones mentioned in claims 5 and 7, to achieve the same effects (resolution and/or sensitivity enhancement). Therefore, the subject matter of claims 5 to 7 does not involve an inventive step (Article 33(3) PCT).

2.2 Document D6

Independent of the above, at least the subject matter of **claims 1 and 7** is not new (Article 33(2) PCT) over the disclosure of D6, because D6 discloses a method as in claim 1 (the "zoom transform"; see, in particular, the first paragraph of section "Zoom transform" and the last paragraph of section "Discussion") applied to spectral data obtained by FT mass spectrometry (FT-MS), i.e. mass spectra.

PATENT COOPERATION TREATY REC'D 2 6 JUL 2006 From the INTERNATIONAL SEARCHING AUTHORITY To: WRITTEN OPINION OF THE see form PCT/ISA/220 INTERNATIONAL SEARCHING AUTHORITY (PCT Rule 43*bis*.1) Date of mailing (day/month/year) see form PCT/ISA/210 (second sheet) Applicant's or agent's file reference FOR FURTHER ACTION see form PCT/ISA/220 See paragraph 2 below International application No. International filing date (day/month/year) Priority date (day/month/year) PCT/EP2005/002114 25.02.2005 19.03.2004 International Patent Classification (IPC) or both national classification and IPC INV. G06F17/14 G01J3/45 **Applicant** THERMO ELECTRON CORPORATION This opinion contains indications relating to the following items: Box No. I Basis of the opinion . ☐ Box No. II **Priority** ☐ Box No. III Non-establishment of opinion with regard to novelty, inventive step and industrial applicability ☐ Box No. IV Lack of unity of Invention Box No. V Reasoned statement under Rule 43bis.1(a)(i) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement ☐ Box No. VI Certain documents cited ☐ Box No. VII Certain defects in the International application Box No. VIII Certain observations on the international application **FURTHER ACTION** If a demand for international prellminary examination is made, this opinion will usually be considered to be a written opinion of the International Preliminary Examining Authority ("IPEA") except that this does not apply where the applicant chooses an Authority other than this one to be the IPEA and the chosen IPEA has notified the International Bureau under Rule 66.1 bis(b) that written opinions of this International Searching Authority will not be so considered. If this opinion is, as provided above, considered to be a written opinion of the IPEA, the applicant is invited to submit to the IPEA a written reply together, where appropriate, with amendments, before the expiration of 3 months from the date of mailing of Form PCT/ISA/220 or before the expiration of 22 months from the priority date, whichever expires later. For further options, see Form PCT/ISA/220. For further details, see notes to Form PCT/ISA/220.

Name and mailing address of the ISA:

D-10958 Berlin

European Patent Office - Gitschiner Str. 103

Tel. +49 30 25901 - 0 Fax: +49 30 25901 - 840 Date of completion of this opinion

see form PCT/ISA/210 **Authorized Officer**

Domingo Vecchioni, M Telephone No. +49 30 25901-666



International application No. PCT/EP2005/002114

_					
_	Box	x No. I Basis of the opinion			
1.	With regard to the language, this opinion has been established on the basis of:				
	⊠ t	the international application in the language in which it was filed			
	□ a	a translation of the international application into , which is the language purposes of international search (Rules 12.3(a) and 23.1 (b)).	ge of a translation furnished for the		
2.	. With regard to any nucleotide and/or amino acid sequence disclosed in the international application and necessary to the claimed invention, this opinion has been established on the basis of:				
	a. type of material:				
		□ a sequence listing			
		□ table(s) related to the sequence listing			
	b. format of material:				
		□ on paper			
		in electronic form			
	c. time of filing/furnishing:				
		\square contained in the international application as filed.			
		illed together with the international application in electronic form.			
		furnished subsequently to this Authority for the purposes of search.			
3.	C	In addition, in the case that more than one version or copy of a sequence has been filed or furnished, the required statements that the information copies is identical to that in the application as filed or does not go beyon appropriate, were furnished.	in the subsequent or additional		
4.	Additional comments:				

International application No. PCT/EP2005/002114

Box No. V Reasoned statement under Rule 43bis.1(a)(i) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement

1. Statement

Novelty (N)

Yes: Claims

5,6

No: Claims

1-4,7-13

Inventive step (IS)

Yes: Claims

No: Claims

Claims

1-13

Industrial applicability (IA)

Yes: Claims

No:

1-13

2. Citations and explanations

see separate sheet

Re Item V

Reasoned statement with regard to novelty, Inventive step or industrial applicability; citations and explanations supporting such statement

- 1. The following documents are cited in the International Search Report:
 - D1: R.T. Pajer and I.M. Armitage: "A method for complex interpolation of spectral segments", *Journal of Magnetic Resonance*, vol. 21, no. 3, March 1976, pages 485-489. [XP002390699]
 - D2: T. Kupka, J. Pacha, and J.O. Dziegielewski: "Application of data processing for sensitivity and resolution enhancement of 31P and 13C NMR spectra of humic substances", *Magnetic Resonance in Chemistry*, vol. 27, no. 1, 1989, pages 21-26. [XP002390700]
 - D3: K. Roth and B. Kirste: "Application of Fourier transformation techniques for sensitivity and resolution enhancement of continuous wave EPR spectra" *Journal of Magnetic Resonance*, vol. 63, no. 2, 15 June 1985, pages 360-364. [XP002390701]
 - D4: J.C. Lindon and A.G. Ferrige: "Digitisation and data processing in Fourier transform NMR", Progress in Nuclear Magnetic Resonance Spectroscopy, vol. 14, 1980, pages 27-66. [XP002390702]
 - D5: Z. Zolnai, J. Juranic, J.L. Markley, and S. Macura: "Zooming, a practical strategy for improving the quality of multidimensional NMR spectra" *Journal of Magnetic Resonance, Series A*, vol. 119, no. 1, March 1996, pages 53-64. [XP002390703]
 - D6: T.J. Francl, R.L. Hunter, and R.T. McIver, Jr. "Zoom transform for mass measurement accuracy in Fourier transform mass spectrometry", *Analytical Chemistry*, vol. 55, no. 13, November 1983, pages 2094-2096. [XP002390704]
 - D7: I. Pelczer and S. Szalma: "Multidimensional NMR and data processing" *Chemical Reviews*, vol. 91, no. 7, November 1991, pages 1507-1524. [XP002390705]

In this communication, reference is made to documents D1 and D6.

- The subject matter of claims 1 to 4 and 7 to 13 is not new in the sense of Article 33(2) PCT.
 The subject matter of claims 5 and 6 appears to be new (Article 33(2) PCT) but does not involve an inventive step in the sense of Article 33(3) PCT.
- 2.1 Document D1

In the wording of the present application, D1 discloses a method (see in particular last paragraph of page 487: the "second method") of enhancing spectral data (see abstract: FT

WRITTEN OPINION OF THE INTERNATIONAL SEARCHING AUTHORITY (SEPARATE SHEET)

International application No.

PCT/EP2005/002114

NMR spectra), said data comprising M discrete intensity values within a range of frequency values ("N point complex spectral segment"), said method comprising:

- applying a first function ("inverse complex transform") being a Fourier transform to the spectral data to obtain an inverse transform of the spectrum ("complex pseudo FID"),
- apodizing said inverse transform ("applying sensitivity or resolution enhancement as desired"; see also page 488, lines 21 to 23: "the pseudo FID is sensitivity enhanced by the function e^{t/r}"),
- zero-filling the apodized inverse transform by a factor Z ("zero extend this pseudo FID by N or more complex points"), and
- applying a second function ("complex transform") to the zero-filled apodized inverse transform to obtain a spectrum comprsing N>M discrete intensities values within said range of frequencies ("interpolated complex spectral segment").

The method is implemented in NMR computer systems (see abstract).

Hence, having regard to the disclosure of D1, the subject matter of claims 1 to 4 and 8 to 13 is not new (Article 33(2) PCT).

The method of D1 is applied to FT NMR spectra. However, it would obvious to a skilled person to use the same method for other kind of spectra, as the ones mentioned in claims 5 and 7, to achieve the same effects (resolution and/or sensitivity enhancement). Therefore, the subject matter of **claims 5 to 7** does not involve an inventive step (Article 33(3) PCT).

2.2 Document D6

Independent of the above, at least the subject matter of claims 1 and 7 is not new (Article 33(2) PCT) over the disclosure of D6, because D6 discloses a method as in claim 1 (the "zoom transform"; see, in particular, the first paragraph of section "Zoom transform" and the last paragraph of section "Discussion") applied to spectral data obtained by FT mass spectrometry (FT-MS), i.e. mass spectra.